Extended Nijboer-Zernike analysis for vectorial diffraction calculations and aberration retrieval

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OUTLINE

- What is the (extended) Nijboer-Zernike analysis?
- Axial extension of the aberrated in-focus diffraction integral to a finite focal region
- Vectorial and high-NA effects
- Future work

What is the Nijboer-Zernike analysis?

- Complete and orthogonal representation of the wavefront aberration in the exit pupil of an optical system using circle polynomials
- Limited to a perfectly spherical support
- First proposed on the unit circle by Szego in 1919
- Introduced in optics by Zernike (1935) and Nijboer (thesis, 1942)

$$W(\rho,\vartheta) = \sum_{n,m} R_n^m(\rho)\left[a_n^m \cos(m\vartheta) + b_n^m \sin(m\vartheta)\right]$$

$$= \sum_{n,m} c_n^m R_n^{|m|}(\rho)\exp(im\vartheta) \qquad (-m_{\max} \le m \le m_{\max})$$

- Immensely popular thanks to Jim Wyant (interferometry) since 1980

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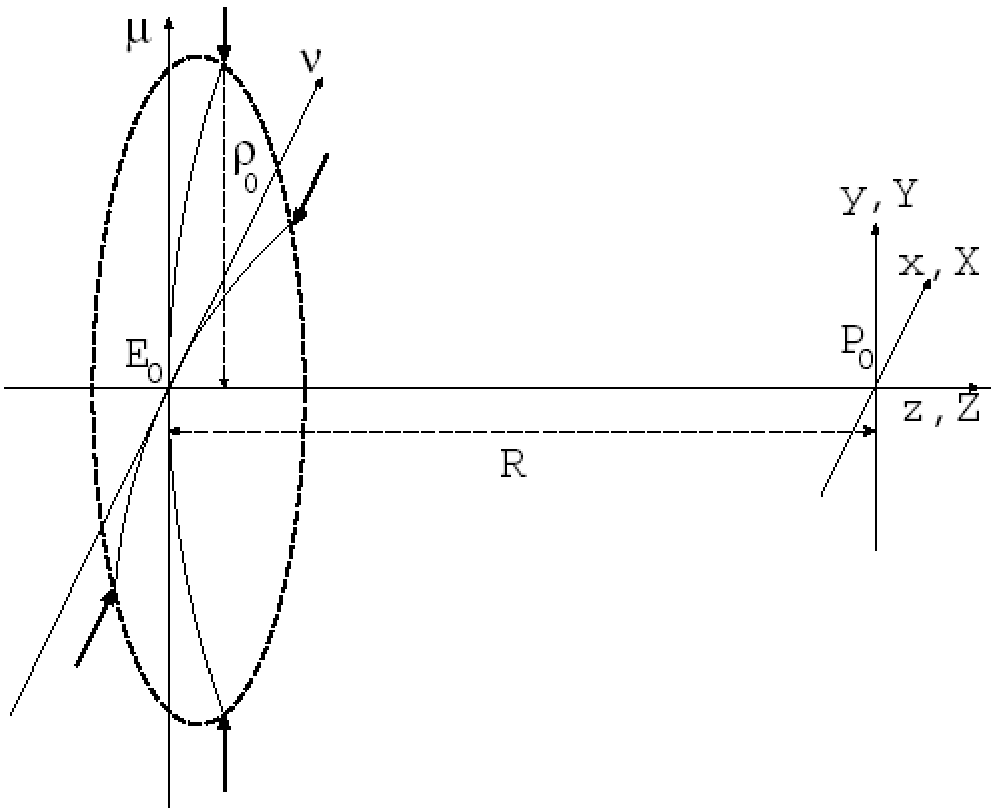
Usefulness of the Nijboer-Zernike analysis

- Optical design:
  The polynomials solve the aberration balancing problem in optical design (Maréchal, Hopkins, Welford: 1940's)
- Diffraction theory:
  Calculation of diffraction patterns for small aberration values and modest defocusing (Nijboer, 1942, Nienhuis, 1943)
- Interferometry:
  Stable reconstruction of measured data;
  'fringe index' of polynomials introduced by Wyant c.s. in 1980
  (37 'first' Zernike polynomials)
- Analytic extension of (aberrated) diffraction integrals to focal *volume* and arbitrary axial position using Zernike polynomials (Janssen, 2002)

Extension through-focus N-Z analysis to high NA values

- Rigorous description of the defocus term, if necessary higher order expansion ($R_4^0(\rho)$ -polynomials etc.)
- Incorporation of vectorial description of focused field for arbitrary state of polarisation
- Inclusion of radiometric effects (Abbe or other imaging conditions)
- Treatment of new (aberrated) diffraction integrals for focal *volume* using Zernike polynomials
  (Braat, Dirksen, Janssen & van de Nes, JOSA A, Dec. 2003)

Standard geometry of focused wave



Coordinates on pupil sphere:

$$\mu + i\nu = \rho \exp(i\vartheta)$$

Coordinates in focal region:

$$r, \varphi, z$$

normalized with respect to:
λ/*NA* (transverse direction *r*)

Defocus parameter *f* in pupil:

$$\Phi_{def} = \frac{2\pi}{\lambda} z \left\{ 1 - \sqrt{1 - \rho^2 (NA)^2} \right\}$$

$$= \frac{f}{1 - \sqrt{1 - (NA)^2}} \left\{ 1 - \sqrt{1 - \rho^2 (NA)^2} \right\}$$

$$\rightarrow \quad f = \frac{2\pi}{\lambda} z \left\{ 1 - \sqrt{1 - (NA)^2} \right\}$$

Diffraction integral (scalar)

$$U(r,\varphi;f)=\frac{1}{\pi}\int_0^1 \rho\exp(if\rho^2)\left[\int_0^{2\pi} A(\rho,\vartheta)\exp\{i\Phi(\rho,\vartheta)\}\times \exp\{i2\pi r\rho\cos(\vartheta-\varphi)\}d\vartheta\right]d\rho$$

Introduction of Zernike polynomials (mapping of amplitude *and* phase):

$$A(\rho,\vartheta)\exp\{i\Phi(\rho,\vartheta)\}=\sum_{n,m}\beta_n^m R_n^{|m|}\exp(im\vartheta)$$

Diffraction integral (scalar)

$$U(r,\varphi;f) = 2\sum_{n,m} i^m \beta_n^m V_n^m(r,f)\cos m\varphi$$

$$V_n^m(r;f) = \int_0^1 \rho \exp(if\rho^2) R_n^m(\rho) J_m(2\pi r\rho) d\rho$$

Analytic solution for the *V* – functions (A.J.E.M. Janssen):

$$V_n^m(r;f) = \exp(if)\sum_{l=1}^{\infty}(-2if)^{l-1}\sum_{j=0}^{p} v_{lj}\,\frac{J_{m+l+2j}(v)}{lv^l};\; p=(n-m)/2, v=2\pi r$$

$$v_{lj} = (-1)^p (m+l+2j)\binom{m+j+l-1}{l-1}\binom{j+l-1}{l-1}\binom{l-1}{p-j}\Big/\binom{q+l+j}{l}; \quad q=(n+m)/2$$

Diffraction integral (scalar)

In-focus Nijboer-Zernike result (1942):

$$U(r,\varphi;0) = 2\left(\frac{J_1(v)}{v} + \sum_{n,m} i^{n+1} \beta_n^m \frac{J_{n+1}(v)}{v} \cos m\varphi \right)$$

Extended (through-focus) result :

$$\mathrm{U}(\mathrm{r},\varphi;\mathrm{f}) = 2\left(\mathrm{V}_0^0(\mathrm{r},\mathrm{f}) + \sum_{\mathrm{n},\mathrm{m}} \mathrm{i}^{\mathrm{m}} \beta_{\mathrm{n}}^{\mathrm{m}} \mathrm{V}_{\mathrm{n}}^{\mathrm{m}}(\mathrm{r},\mathrm{f}) \cos \mathrm{m}\varphi \right)$$

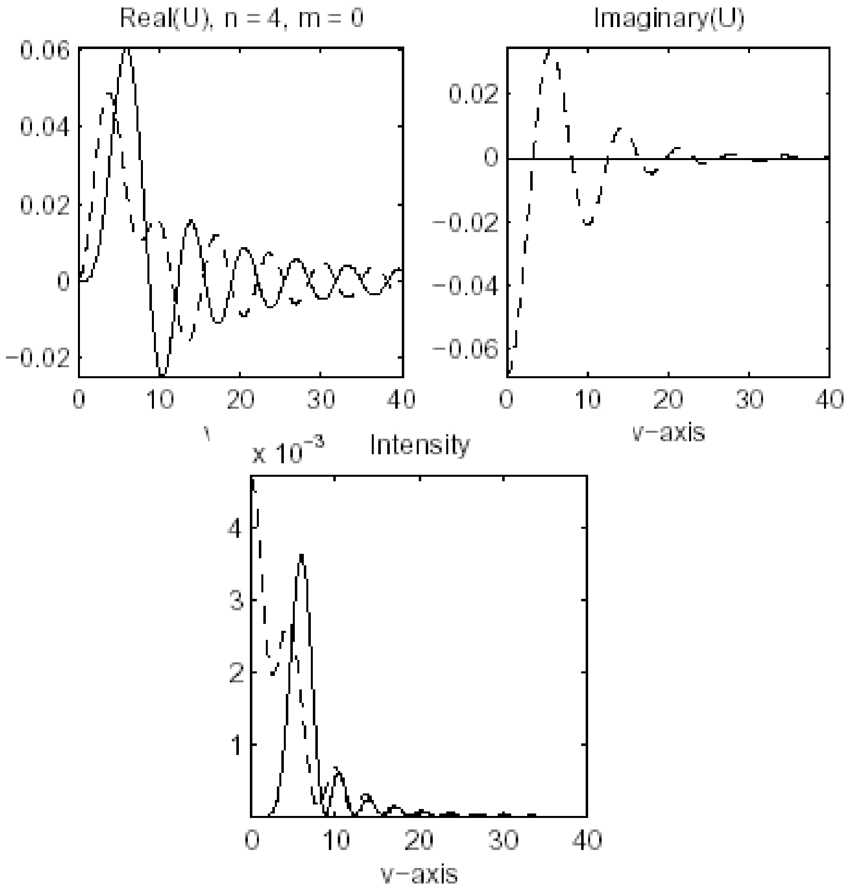
Convergence conditions:

$$L = l_{\max} = 25 \qquad \text{for :}$$

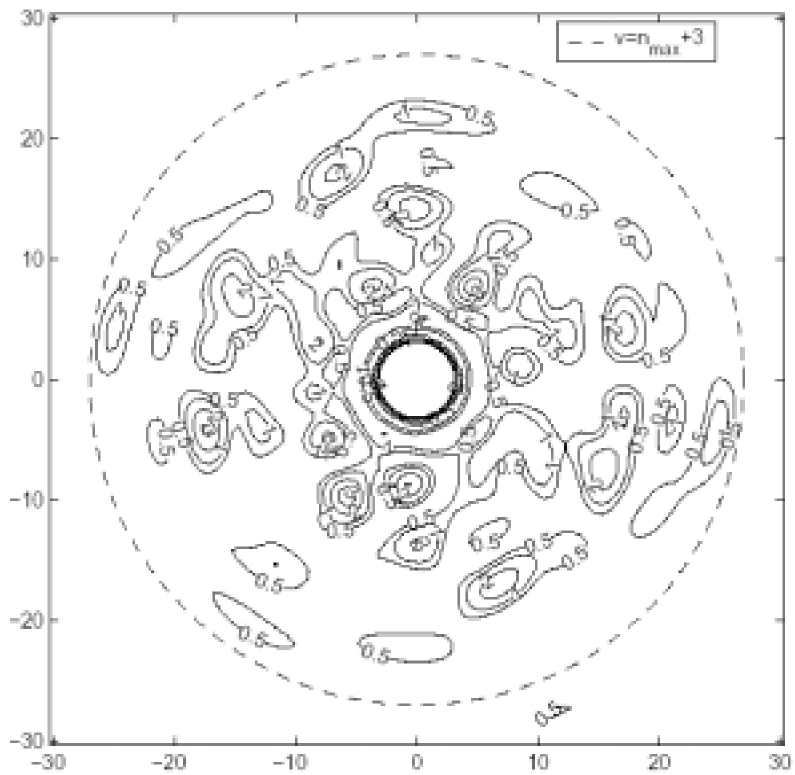
$$|\, f\,| \le 2\pi, \quad v = 2\pi r \le 20, \quad 0 \le p \le q \le 6, \text{abs. error} \le 10^{-6}$$

Some calculated patterns

Re{$V_{4,0}$}, Im{$V_{4,0}$} and $|V_{4,0}|^2$



High-frequent pupil ‘noise’; intensity pattern image plane



Extension to high-NA case

1) Correct treatment of defocus-parameter: $$\exp\left(-\frac{if}{u_0}\sqrt{1-s_0^2\rho^2}\right)$$
$$\left(u_0 = 1-\sqrt{1-s_0^2}\right)$$

2) Inclusion of 'radiometric' effect
(aplanatic system with magnification M=0): $$\frac{1}{\left(1-s_0^2\rho^2\right)^{1/4}}$$

3) Finite-size point-source
(accounted for by Gaussian pupil 'transmission'): $$\exp\left(-\tilde{f}\rho^2\right)$$

a complex defocus parameter $f_C = f + i\tilde{f}$
is used!

4) Higher than quadratic effects are 'stored' in symmetrical polynomials of order *2n* leading to the formal expression at high NA: $$\exp\left(g + f_C\rho^2\right)\sum_{k=0}^{k_{max}} h_k R_{2k}^0(\rho)$$

Extension to vectorial treatment

The Ignatowsky / Richards & Wolf treatment of the ***aberrated*** case leads to three diffraction integrals that recall the I_0-, $I_1-$and I_2-integrals

$$\vec{E}^x(r,\varphi;f) = -i\gamma s_0^2 \exp\left(\frac{-if}{1-\sqrt{1-s_0^2}}\right)\sum_{n,m} i^m \beta_n^{m,x} \exp(im\varphi)\times$$

$$\begin{pmatrix} V_{n,0}^m + \frac{s_0^2}{2}V_{n,2}^m \exp(2i\varphi) + \frac{s_0^2}{2}V_{n,-2}^m \exp(-2i\varphi) \\ -\frac{is_0^2}{2}V_{n,2}^m \exp(2i\varphi) + \frac{is_0^2}{2}V_{n,-2}^m \exp(-2i\varphi) \\ -is_0 V_{n,1}^m \exp(i\varphi) + is_0 V_{n,-1}^m \exp(-i\varphi) \end{pmatrix}$$

Each aberration term creates its own $V_{n,0}^m$ and $V_{n,k}^m \exp(ik\varphi)$ terms $(k = \pm 1, \pm 2)$.

New integral *V* to be treated

Old $V_n^m(r, f)$ - integral (scalar treatment)

$$V_n^m(r, f) = \int_0^1 \exp\left[if\rho^2\right] R_n^{|m|}(\rho) J_m(2\pi r\rho)\, \rho d\rho$$

New $V_{n,j}^m(r, f)$ - integral (vectorial treatment):

$$V_{n,j}^m(r, f) = \int_0^1 \rho^{|j|} \left(1 + \sqrt{1 - s_0^2\rho^2}\right)^{-|j|+1} \exp\left[\frac{if}{1 - \sqrt{1 - s_0^2}} \left(1 - \sqrt{1 - s_0^2\rho^2}\right)\right] \times$$

$$R_n^{|m|}(\rho) J_{m+j}(2\pi r\rho)\, \rho d\rho$$

The second integral can be treated using the analytic series expansion solution of $V_n^m(r, f)$

Results of analytic vectorial analysis (no aberrations)

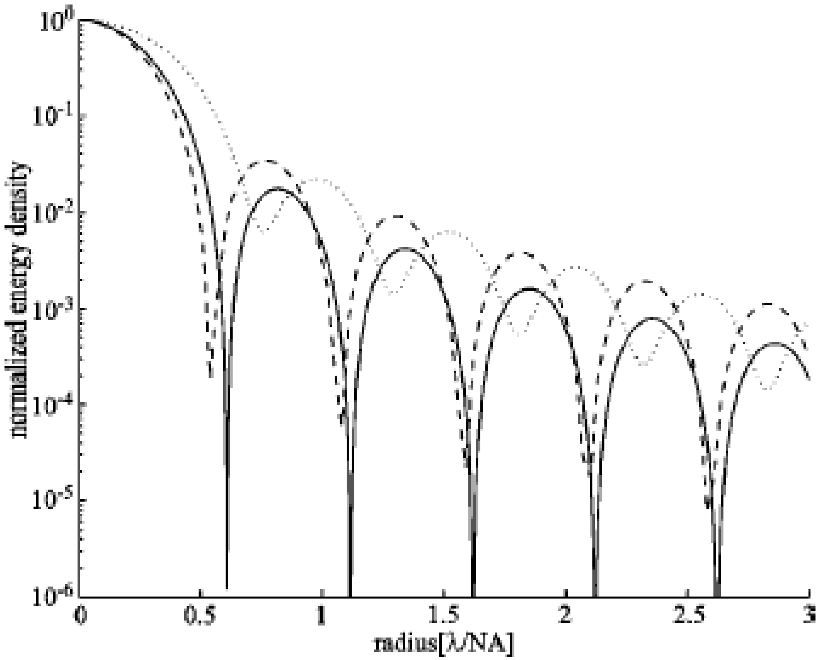


Fig. 3. Comparison of the energy density function in the high-NA focus ($f = 0$) and the scalar Airy distribution as a function of the radial coordinate r. The energy density function in the cross section $\theta = 0$ is represented by the dotted curve, and the one in the cross section $\theta = \pi/2$ by the dashed curve. The scalar Airy distribution is shown by the solid curve. The fact that the dashed high-aperture curve does not reach very low levels is due to the sampling density used in plotting this curve.

Comparison of scalar (Airy-disc) intensity cross-section and vectorial cases:

- $\theta = 0$
- $\theta = \pi / 2$

Introduction of aberrations

The complex pupil function is written as

$$B^x(\rho,\vartheta) = A^x(\rho,\vartheta)\exp\left[i2\pi W(\rho,\vartheta)\right]$$

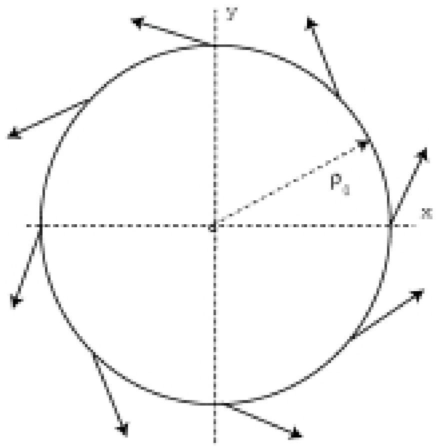
$$B^y(\rho,\vartheta) = A^y(\rho,\vartheta)\exp\left[i2\pi W(\rho,\vartheta) + i\varepsilon(\rho,\vartheta)\right]$$

A is the transmission function, W the wavefront aberration and ε the (phase) birefringence

Special types of polarisation : RADIAL

$$A^x = A_0 \cos(\vartheta + \vartheta_0)$$

$$A^y = A_0 \sin(\vartheta + \vartheta_0)$$



Radiometric effect and Zernike expansion

The complex pupil function including the radiometric effect is written as

$$B_R^x(\rho,\vartheta)=\frac{B^x(\rho,\vartheta)}{\left(1-s_0^2\rho^2\right)^{1/4}}\exp\left[i2\pi W(\rho,\vartheta)\right]=\sum_{n,m}\beta_n^{m,x}R_n^{|m|}(\rho)\exp\left[im\vartheta\right]$$

s_0 is the numerical aperture; m runs from $-m_{\max}$ to $+m_{\max}$.

The $\beta_n^{m,x}$ are calculated as usually following

$$\beta_n^{m,x}=\frac{n+1}{\pi}\int_0^1\int_0^{2\pi}\frac{B^x(\rho,\vartheta)}{\left(1-s_0^2\rho^2\right)^{1/4}}R_n^{|m|}(\rho)\exp\left[-im\vartheta\right]\rho d\rho d\vartheta$$

with normalisation according to

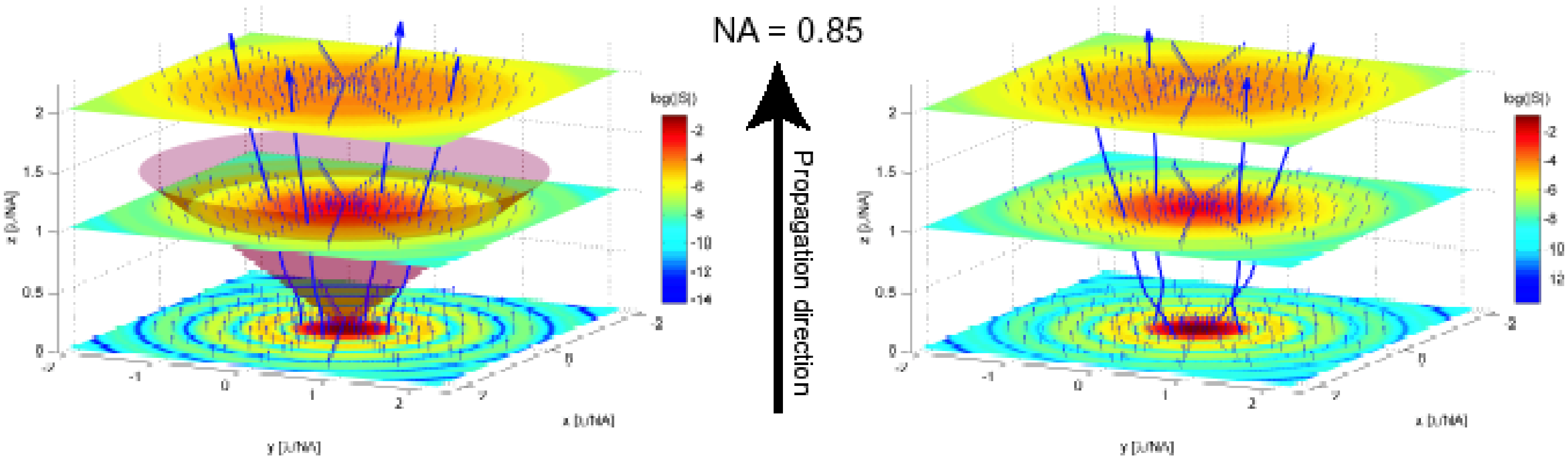
$$\int_0^1 R_{n'}^{|m|}(\rho)R_n^{|m|}(\rho)\rho d\rho=\frac{\delta_{nn'}}{2(n+1)}$$

Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
(using the analytic expression for the Poynting vector)

Linearly polarised light

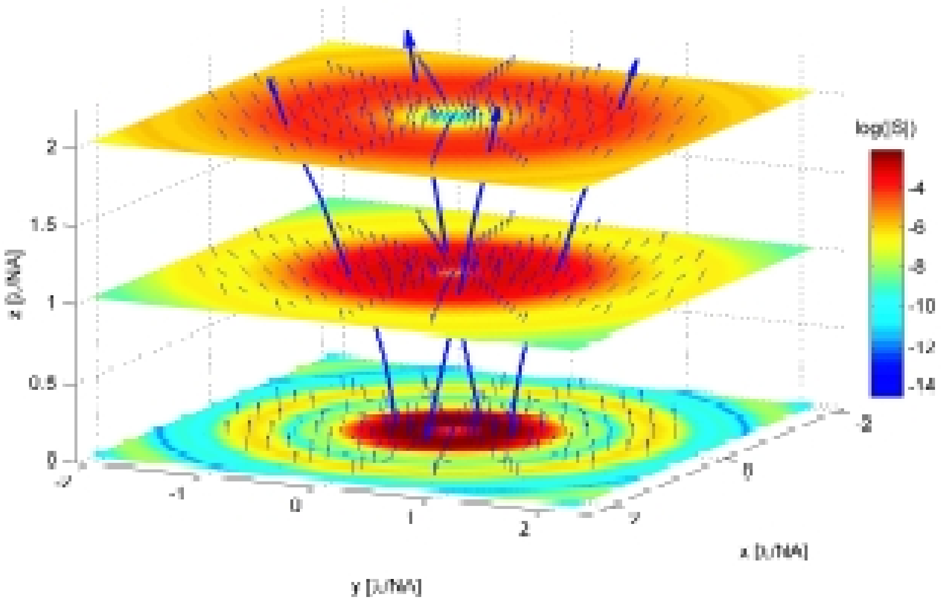
Right circularly polarized light



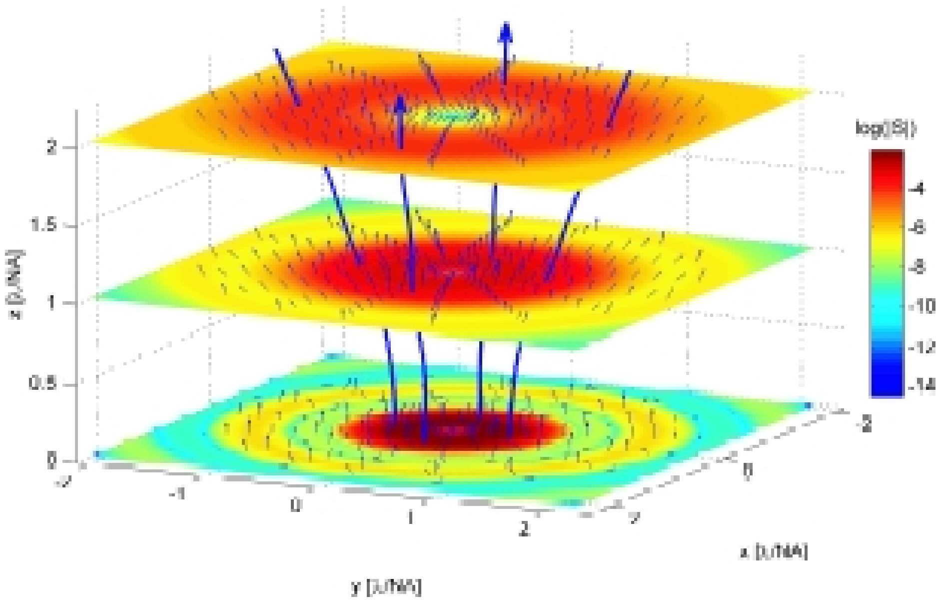
Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
(using the analytic expression for the Poynting vector)

Orbital angular momentum (l=1)



OAM (l=1) + right circularly polarised light



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Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
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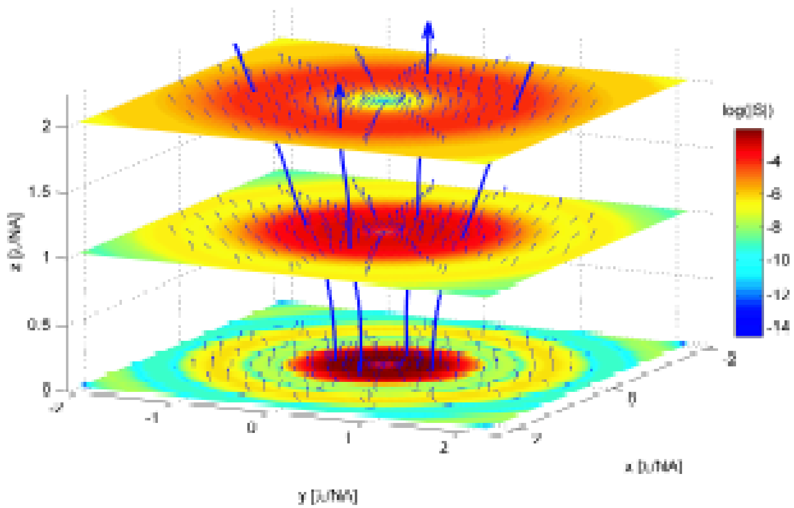
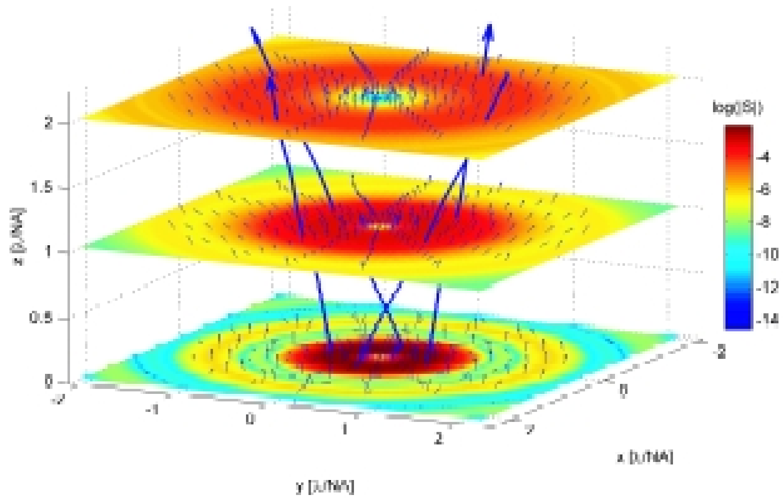
Orbital angular momentum (l=1)
+ right circular polarisation



Orbital angular momentum (l=1)
+ left circular polarisation



How to obtain a parametric expression for the field density in the imaging volume?

$$w_E = \frac{\varepsilon_0}{4} n_r^2 |E|^2 = \frac{\varepsilon_0}{4} n_r^2 \left\{ E_1 E_1^* + E_2 E_2^* + E_3 E_3^* \right\} \text{with :}$$

$$\vec{E}^x(r,\varphi; f) = -i\gamma s_0^2 \exp\left(\frac{-if}{1-\sqrt{1-s_0^2}} \right) \sum_{n,m} i^m \beta_n^{m,x} \exp(im\varphi) \times$$

$$\left(\begin{array}{c} V_{n,0}^m + \frac{s_0^2}{2} V_{n,2}^m \exp(2i\varphi) + \frac{s_0^2}{2} V_{n,-2}^m \exp(-2i\varphi) \\ -\frac{is_0^2}{2} V_{n,2}^m \exp(2i\varphi) + \frac{is_0^2}{2} V_{n,-2}^m \exp(-2i\varphi) \\ -is_0 V_{n,1}^m \exp(i\varphi) + is_0 V_{n,-1}^m \exp(-i\varphi) \end{array} \right)$$

$$dW_{\exp} = \frac{\partial w_E}{\partial t} \Delta t \text{ is the quantity that determines the resist exposure per unit volume in time } \Delta t!$$

Basic term in the expression for the exposure

$$G_{kl}(r,\varphi;f)=$$

$$\sum_{n,m} i^m \alpha_n^m V_{n,k}^m \exp(im\varphi)\exp(ik\varphi)\times\sum_{n',m'} i^{-m'}\beta_{n'}^{m'} V_{n',l}^{m'*}\exp(-im'\varphi)\exp(-il\varphi)=$$

$$\sum_{n',m'}\exp\{i(m-m')\pi/2\}\exp\{i(m-m'+k-l)\varphi\}\alpha_n^m\beta_{n'}^{m'*}V_{n,k}^m(r,f)V_{n',l}^{m'*}(r,f)$$

Small β - approximation (dominating β_0^0 - coefficient)

$$G_{kl}(r,\varphi;f)=e^{i(k-l)\varphi}\sum_{\nu=0}^{\nu_{\max}}\sum_{\mu=-\mu_{\max}(\nu)}^{+\mu_{\max}(\nu)}\left\{\begin{array}{l} e^{-i\mu\pi/2}e^{-i\mu\varphi}\alpha_0^0\beta_\nu^{\mu*}V_{0,k}^0(r,f)V_{\nu,l}^{\mu*}(r,f)+ \\ \qquad (1-\varepsilon_{\nu\mu})e^{+i\mu\pi/2}e^{+i\mu\varphi}\alpha_\nu^\mu\beta_0^{0*}V_{\nu,k}^\mu(r,f)V_{0,l}^{0*}(r,f)\end{array}\right\}$$

Representation of light intensity (fully polarised case)

$$\beta_n^{m,x} = a\beta_n^m$$

$$\beta_n^{m,y} = b\beta_n^m$$

$(|a|^2 + |b|^2 = 1$ for normalisation purposes)

$$w_E(r,\varphi;f) = \frac{\varepsilon_0 n_r^2 s_0^2}{4}\left[\begin{array}{l} G_{00}(\beta,\beta) + \\ s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{0,2}(\beta,\beta)\right\} - 2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\left\{G_{0,2}(\beta,\beta)\right\}\right\} + \\ s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{0,-2}(\beta,\beta)\right\} + 2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\left\{G_{0,-2}(\beta,\beta)\right\}\right\} + \\ \dfrac{s_0^4}{2}\left\{\left[1 - 2\,\mathrm{Im}(ab^*)\right]G_{2,2}(\beta,\beta) + \left[1 + 2\,\mathrm{Im}(ab^*)\right]G_{-2,-2}(\beta,\beta)\right\} + \\ s_0^2\left\{\left[1 - 2\,\mathrm{Im}(ab^*)\right]G_{1,1}(\beta,\beta) + \left[1 + 2\,\mathrm{Im}(ab^*)\right]G_{-1,-1}(\beta,\beta)\right\} + \\ -2s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{+1,-1}(\beta,\beta)\right\} + 2\,\mathrm{Re}(ab^*)\,\mathrm{Im}\left\{G_{+1,-1}(\beta,\beta)\right\}\right\} \end{array}\right]$$

Strehl intensity

On – axis (Srehl) intensity using β - type expansion

$$\mathrm{A_S} = \frac{1}{\pi}\int_0^{2\pi}\int_0^1 B(\rho,\vartheta)\rho d\rho d\vartheta =$$

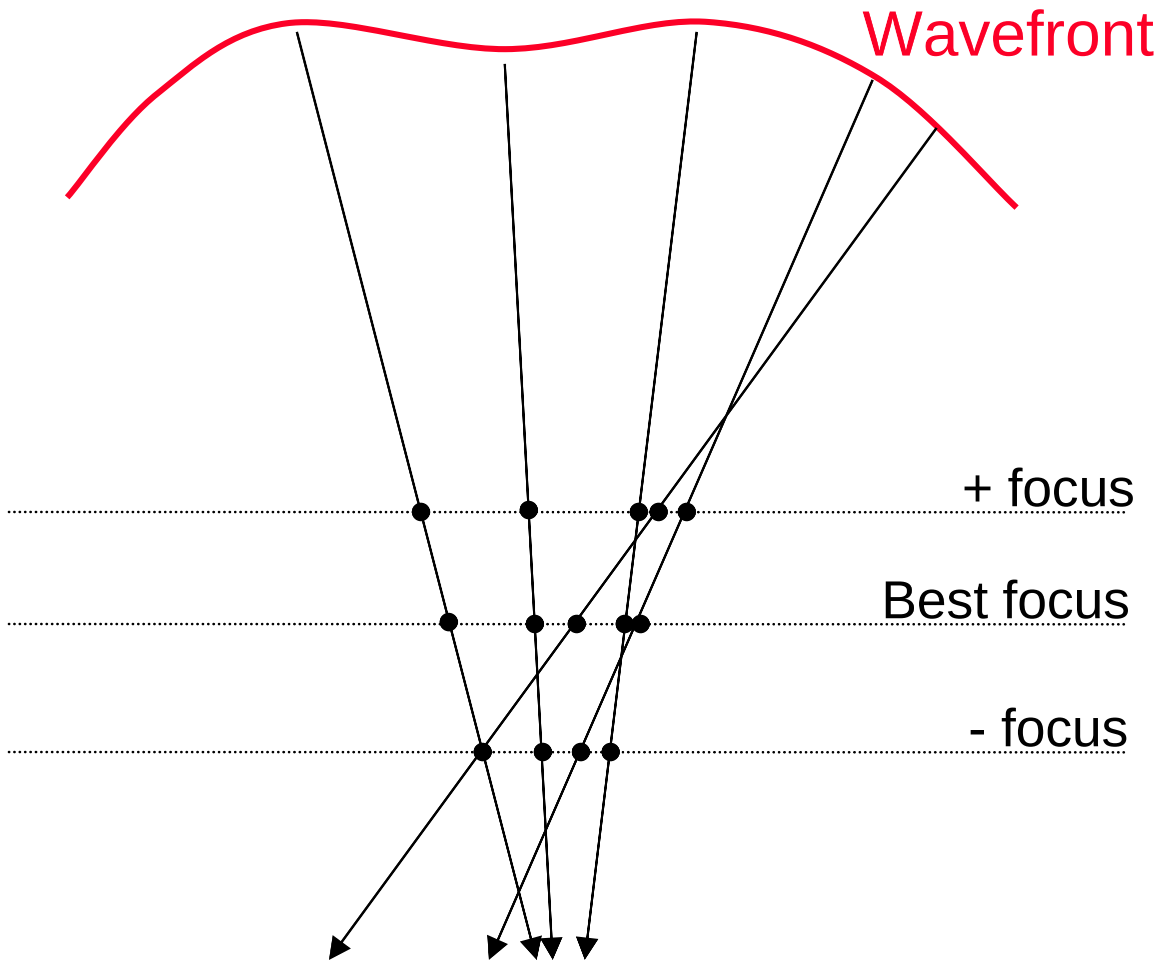
$$\frac{1}{\pi}\int_0^{2\pi}\int_0^1 \sum_{n,m}\beta_n^m R_n^m(\rho)\exp(im\vartheta)\rho d\rho d\vartheta =$$

$$\sum_{n,m}\beta_n^m \frac{1}{\pi}\int_0^{2\pi}\int_0^1 R_n^m(\rho)\exp(im\vartheta)\rho d\rho d\vartheta = \beta_0^0$$

$$\rightarrow I_S = \left|\beta_0^0\right|^2 \quad \text{(scalar approximation)}$$

With the radiometric effect included in the Zernike expansion, the relation remains true also in the vectorial case!

Complex pupil function reconstruction remains possible in the vectorial case?



Intuitive picture of aberration retrieval

Further developments

- Complex amplitude retrieval of the pupil function at large NA should remain possible thanks to the parametric description of the intensity distribution in the focal volume using the Zernike ß-expansion and the extended Nijboer-Zernike theory applied to the vectorial diffraction.

- Much of the numerical work in solving the system of equations for the ß-coefficients has to be done only once and the results can be tabulated and stored for further use.

- Simultaneous retrieval of aberration and birefringence possible?